Supporting information for

Solvent Dependent Assembly and Dis-assembly of Hydrogen Bonded Helical Structure in a Co-Mo Bimetallic Complex

Snehadrinarayan Khatua[†], Takunori Harada[§], Reiko Kuroda[§], and Manish Bhattacharjee[†]*

[†]*Department of Chemistry, Indian Institute of Technology, Kharagpur 721 302, India.* [§]*Department of Life Sciences, Graduate School of Arts and Sciences, University of Tokyo, Komaba, Meguro-ku, Tokyo 153-89021, Japan*

Materials and Physical Measurements.

The chemicals used were obtained from the following sources:

2,4-di-*tert*-butyl phenol was purchased from Fluka. Glycine, formaldehyde, $Na_2MoO_4.2H_2O$ and solvents used were reagent grade products.

The elemental analyses (C, H, N) were performed with a Perkin-Elmer model 240 C elemental analyzer. IR spectra were recorded on a Perkin-Elmer 883 spectrophotometer. ^{1}H NMR spectra of the ligand were recorded on a Bruker Avance II 400 MHz spectrometer. The powder X-ray diffraction (PXRD) pattern for compound **1** and **2** were recorded in an X'pert pro diffractometer with Co (K_α= 1.78891) radiation and were then converted to the pattern with Cu (K_α= 1.54178) source. The solution electronic spectra were obtained using a Shimadzu UV 3100 UV-vis-NIR spectrophotometer respectively. Solid state transmittance CD spectra were measured as KBr discs on the purpose-built JASCO J800 KCM spectrophotometer,[1] and were corrected for artifacts arising from linear dichroism and linear birefringence. The diffuse reflectance (DRCD) spectra of powdered samples were recorded on powdered samples on a quartz plate. The ligand was synthesized by a modified reported procedure[2] and characterized by elemental analyses, IR, UV-visible and ^{1}H NMR ($CDCl_3$).

Synthesis of the bimetallic cobalt complexes 1, 2 and 3.

Synthesis of [{$(MoO_2L)_2Co(H_2O)_6$}$^{\cdot}$$3H_2O$] (1): An aqueous solution of Na_2MoO_4, $2H_2O$ (0.2419 gm, 1mmol) was added to the aqueous methanolic solution of Na_2HL (0.396g, 1mmol) and pH was adjusted to 5-6 by adding dil HCl. After 6 hours stirring at room temperature an aqueous solution of $CoCl_2{\cdot}6H_2O$ (0.7131g, 3 mmol) was added to the reaction mixture and stirring was continued for further 1 hour. The pH of the reaction solution was found to be 3 at this stage. The reaction mixture was allowed to stand in air for one week where upon an orange yellow crystalline solid separated. The solid was then washed with water and dried under air. Yield: 68 %. C, H, N analysis calc.(%) for $C_{38}H_{70}CoMo_2N_2O_{23}$ (M = 1173.78 gmol^{-1}): C 38.88, H 6.01, N 2.39; found: C 38.96, H 5.98, N 2.41. FTIR in KBr disc (ν_{max} /cm^{-1}): 3395; 1618; 1391; 1236; 900 and 857. Uv-visible (λ_{max}): 376(8117), 259(15647).

Synthesis of [{$(MoO_2L)Co(H_2O)_4(MeOH)$}{MoO_2L}]$^{\cdot}$$2H_2O^{\cdot}MeOH$, (2) : The compound **1** was synthesized by the above procedure and was dried under vacuum. Compound **1** was redissolved in pure MeOH. The Methanolic solution on standing for 4-5 days afforded deep red colored crystal of **2a** (**2a** and **2b** are two enantiomorphs) suitable for X-ray diffraction. Yield: 42%. C, H, N analysis (crystal) calc.(%) for $C_{40}H_{72}CoMo_2N_2O_{22}$ (M = 1183.81 gmol^{-1}): C 40.58, H 6.13, N 2.37; found: C 40.62, H 6.06, N 2.34. FTIR in KBr disc (ν_{max} /cm^{-1}): 3411; 1620 1390; 1237; 901 and 857. Uv-visible (λ_{max}): 374(7287), 258(13117).

NOTE: Normally, *P*-helical isomer (**2a)** crystallized first. We have checked this for five different batches of reactions. The crystals were separated and the mother liquor on standing afforded the crystals of *M*-helical isomer. Crystals of *M*-helical isomer **(2b)** were selectively obtained when, a small amount D-glucose (compound: D-glucose = 10 : 1) is added to the methanolic solution of **1.**

Synthesis of [{$(MoO_2L)_2Co(H_2O)_4$}{$(MoO_2L)_2Co(H_2O)_6$}]$^{\cdot}$$4H_2O^{\cdot}2^{i}PrOH$ (3): Recrystallization of vacuum-dried **1** from 2-Propanol afforded orange red crystals of **3**

suitable for X-ray structure analysis. Yield: 34%; C, H, N Calc. (%) for $C_{82}H_{148}Co_2Mo_4N_4O_{44}$ (M = 2395.68 gmol^{-1}): C 41.11, H 6.23, N 2.34; found: C 41.21, H 6.18, N 2.35. FTIR in KBr disc (ν_{max} /cm^{-1}): 3432; 2960; 1626 1389; 1238; 910 and 858. UV-visible (λ_{max}): 376(7882), 259(15572).

Crystallographic Structure Determinations

The single crystal data of compounds **1, 2(a** and **b),** and **3** were collected on Bruker-Nonius Mach3 CAD4 X-ray diffractometer that uses graphite monochromated Mo Kα radiation (λ = 0.71073 Å) by ω-scan method. The structures were solved by SIR-92[3] (**11a 11b** and **12**) and by Direct methods using the program SHELXS-97[4] (**10**) and refined by least square methods on F^2 using SHELXL-97.[5] Non-hydrogen atoms were refined anisotropically (except O5W in **2a** and O40A and O40B in **2b**) and hydrogen atoms on C-atoms were fixed at calculated positions and refined using a riding model. Whereas H-atoms on water molecules and coordinated methanol oxygen (only for **2a** and **2b**) in **1, 2** (**a** and **b)** and **3** could not be located. No absorption correction was used for compound **2a, 2b** and **3**. For compound **1** an absorption correction was applied by using the program XABS2[6] and the maximum and minimum transmission factors 0.9191 and 0.6737. In **1**, three C atoms, C13, C14 and C15 were disordered and splitted over two positions (C13A, C13B and C14A, C14B and C15A C15B). The occupancy of each C atom was set to 50%. Three DFIX restraints [d_{C-C} = 1.53(2)Å] were applied for three C-C distances (C12-C15A, C12- C14A and C12-C13A). Other DFIX restraint [d_{C-C} = 1.50(2)Å] were applied for C-C distances (C14A-C13A) Hydrogen atoms on the disordered C-atoms were not fixed. The details of crystal data of **1, 2a**, **2b** and **3** are given in Table 1-3. The selected bond lengths and bond angles are given in Table 4 to Table 7. Structures were drawn by ORTEP[7] and PLUTON[8] program.

Table 1: Crystal data for 1

Empirical formula	$C_{38}H_{70}CoMo_2N_2O_{23}$
Formula weight	1173.77
Temperature, K Wavelength (Å)	293(2), 0.71073
Crystal system, Space group	Monoclinic, $P2_1/a$
Unit cell dimensions	
a (Å)	12.156(9)
b (Å)	9.139(7)
c (Å)	23.765(12)
α (°)	90
β(°)	95.00(9)
γ(°)	90
V ($Å^3$)	2630(3)
Z	2
$\rho_{calcd.}$ (Mg/m^3)	1.482
μ (mm^{-1})	0.858
F(000)	1214
Crystal size (mm)	0.50 x 0.30 x 0.10
θ Range (°)	1.72 to 24.98
Reflections collected	5192
Independent reflections	4767 [R(int) = 0.000]
Absorption correction	Empirical (XABS2)
T_{max}, T_{min}	0.9191, 0.6737
Data / restraints / parameters	4767 / 4 / 334
Goodness-of-fit on F^2	1.097
Final R indices [I>2σ(I)]	R1 = 0.1036, wR2 = 0.2681
R indices (all data)	R1 = 0.1855, wR2 = 0.3244
Diffractometer	CAD4-MACH3

Table 2: Crystal data for 2a and 2b

	2a	**2b**
Empirical formula	$C_{40}H_{72}CoMo_2N_2O_{22}$	$C_{40}H_{72}CoMo_2N_2O_{22}$
Formula weight	1183.81	1183.81
Temperature, K	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system, Space group	Monoclinic, $P2_1$	Monoclinic, $P2_1$
Unit cell dimensions		
a (Å)	13.735(3)	13.792(2)
b (Å)	11.7385(11)	11.692(2)
c (Å)	16.8051(11)	16.692(5)
α (°)	90	90
β(°)	96.542(9)	96.428(8)
γ(°)	90	90
V ($Å^3$)	2691.9(6)	2674.8(10)
Z	2	2
ρ_{calcd} (Mg/m^3)	1.461	1.452
μ (mm^{-1})	0.837	0.842
F(000)	1226	1226
Crystal size (mm)	0.20 x 0.20 x 0.10	0.50 x 0.35 x 0.20
θ Range (°)	1.22 to 24.97	1.23 to 24.97
Reflections collected	5203	5161
Independent reflections	4980 [R(int) = 0.0097]	4944[R(int) = 0.0265]
Absorption correction	none	none
Data / restraints / parameters	4980 / 2 / 614	4944 / 1 / 616
Goodness-of-fit on F^2	1.085	1.065
R1, wR2 Final [I>2σ(I)]	0.0421, 0.1060	0.0525, 0.1084
R1, wR2 (all data)	0.0528, (0.1124)	0.1252, (0.1282)
Diffractometer	CAD4-MACH3	CAD4-MACH3
Absolute structure parameter	-0.01(3)	0.01(4)

Table 3 Crystal data for 3

Empirical formula	$C_{82}H_{148}Mo_4N_4Co_2O_{44}$
Formula weight	2395.68
Temperature, K	293(2)
Wavelength (Å)	0.71073
Crystal system, Space group	Triclinic, *P*-1
Unit cell dimensions	
a (Å)	10.1258(15)
b (Å)	13.035(17)
c (Å)	22.385(10)
α (°)	73.785(3)
β (°)	77.951(3)
γ(°)	81.569(11)
V (Å^3)	2781.5(13)
Z	1
ρ_{calcd} (Mg/m^3)	1.430
μ (mm^{-1})	0.811
F(000)	1242
Crystal size (mm)	0.50 x 0.30 x 0.20
θ Range (°)	1.63 to 24.97
Reflections collected	10383
Independent reflections	9771 [R(int) = 0.0262]
Data / restraints / parameters	9771 / 1 / 631
Goodness-of-fit on F^2	1.090
Final R indices [I>2σ(I)]	R1 = 0.0560, wR2 = 0.1624
R indices (all data)	R1 = 0.0961, wR2 = 0.1807
Diffractometer	CAD4-MACH3

Table 4: The bond lengths (Å) and bond angles around Mo and Co center in compound 1.

Mo(1)-O(1)	1.867(8)	Mo(1)-O(2)	1.708(8)
Mo(1)-O(3)	1.669(9)	Mo(1)-O(4)	2.054(10)
Mo(1)-O(6)	2.203(9)	Mo(1)-N(1)	2.347(9)
Co(1)-O(1W)	2.135(8)	Co(1)-O(1W)#1	2.135(8)
Co(1)-O(2W)	2.070(8)	Co(1)-O(2W)#1	2.070(8)
Co(1)-O(3W)	2.108(10)	Co(1)-O(3W)#1	2.108(10)

Angles around Mo-center

O(1)-Mo(1)-O(4)	153.3(3)	O(1)-Mo(1)-O(6)	84.3(4)
O(2)-Mo(1)-O(1)	105.2(4)	O(2)-Mo(1)-O(4)	95.1(4)
O(2)-Mo(1)-O(6)	88.1(4)	O(3)-Mo(1)-O(1)	100.2(5)
O(3)-Mo(1)-O(2)	106.9(5)	O(3)-Mo(1)-O(4)	90.0(5)
O(3)-Mo(1)-O(6)	162.4(4)	O(4)-Mo(1)-O(6)	79.3(4)
O(1)-Mo(1)-N(1)	79.7(3)	O(2)-Mo(1)-N(1)	158.7(5)
O(3)-Mo(1)-N(1)	92.3(4)	O(4)-Mo(1)-N(1)	75.3(3)

Angles around Co- center

O(1W)-Co(1)-O(1W)#1	180.0(6)	O(2W)-Co(1)-O(2W)#1	180.00(1)
O(3W)-Co(1)-O(3W)#1	180.00(13)	O(2W)-Co(1)-O(3W)	88.0(4)
O(2W)-Co(1)-O(1W)	87.8(3)	O(3W)-Co(1)-O(1W)	90.7(4)
O(2W)-Co(1)-O(1W)#1	92.2(3)	O(2W)-Co(1)-O(3W)#1	92.0(4)
O(2W)#1-Co(1)-O(3W)	92.0(4)	O(2W)#1-Co(1)-O(3W)#1	88.0(4)
O(2W)#1-Co(1)-O(1W)	92.2(3)	O(2W)#1-Co(1)-O(1W)#1	87.8(3)
O(3W)-Co(1)-O(1W)#1	89.3(4)	O(3W)#1-Co(1)-O(1W)	89.3(4)
O(3W)#1-Co(1)-O(1W)#1	90.7(4)	C(10)-N(1)-Mo(1)	108.5(6)
C(8)-N(1)-Mo(1)	109.2(6)	C(7)-N(1)-Mo(1)	107.4(7)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

Table 5: The bond lengths (Å) and bond angles around Mo and Co center in compound 2a

Mo(1)-O(1)	1.683(5)	Mo(1)-O(2)	1.681(5)
Mo(1)-O(3)	1.904(5)	Mo(1)-O(4)	2.098(5)
Mo(1)-O(6)	2.186(5)	Mo(2)-O(8)	1.712(6)
Mo(2)-O(9)	1.697(5)	Mo(2)-O(10)	1.887(5)
Mo(2)-O(11)	2.040(5)	Mo(2)-O(13)	2.218(6)
Mo(1)-N(1)	2.345(5)	Mo(2)-N(2)	2.335(6)
Co(1)-O(1W)	2.157(11)	Co(1)-O(2W)	2.080(7)
Co(1)-O(3W)	2.114(6)	Co(1)-O(4W)	2.069(8)
Co(1)-O(20)	2.089(11)	Co(1)-O(7)	2.093(6)

Angles around Mo-center

O(2)-Mo(1)-O(1)	105.9(3)	O(2)-Mo(1)-O(3)	98.9(2)
O(1)-Mo(1)-O(3)	104.7(3)	O(2)-Mo(1)-O(4)	90.2(2)
O(1)-Mo(1)-O(4)	95.3(3)	O(3)-Mo(1)-O(4)	154.70(19)
O(2)-Mo(1)-O(6)	162.7(2)	O(1)-Mo(1)-O(6)	89.8(2)
O(3)-Mo(1)-O(6)	83.9(2)	O(4)-Mo(1)-O(6)	80.8(2)
O(2)-Mo(1)-N(1)	91.3(2)	O(1)-Mo(1)-N(1)	158.5(2)
O(3)-Mo(1)-N(1)	84.84(19)	O(4)-Mo(1)-N(1)	71.33(18)
O(6)-Mo(1)-N(1)	71.87(17)	O(9)-Mo(2)-O(8)	105.7(3)
O(9)-Mo(2)-O(10)	98.8(3)	O(8)-Mo(2)-O(10)	102.2(3)
O(9)-Mo(2)-O(11)	91.1(2)	O(8)-Mo(2)-O(11)	96.8(3)
O(10)-Mo(2)-O(11)	155.3(2)	O(9)-Mo(2)-O(13)	162.4(3)
O(8)-Mo(2)-O(13)	90.7(3)	O(10)-Mo(2)-O(13)	83.6(2)
O(11)-Mo(2)-O(13)	80.5(2)	O(9)-Mo(2)-N(2)	89.9(3)
O(8)-Mo(2)-N(2)	162.0(3)	O(10)-Mo(2)-N(2)	83.5(2)
O(11)-Mo(2)-N(2)	73.8(2)	O(13)-Mo(2)-N(2)	72.9(2)

Angle around Co center

O(4W)-Co(1)-O(2W)	175.2(5)	O(4W)-Co(1)-O(20)	92.8(5)
O(2W)-Co(1)-O(20)	90.8(5)	O(4W)-Co(1)-O(7)	93.8(2)
O(2W)-Co(1)-O(7)	89.4(3)	O(20)-Co(1)-O(7)	90.2(3)
O(4W)-Co(1)-O(3W)	85.8(3)	O(2W)-Co(1)-O(3W)	91.1(3)
O(20)-Co(1)-O(3W)	88.1(3)	O(7)-Co(1)-O(3W)	178.2(3)
O(4W)-Co(1)-O(1W)	88.2(5)	O(2W)-Co(1)-O(1W)	88.2(5)
O(20)-Co(1)-O(1W)	178.9(5)	O(7)-Co(1)-O(1W)	89.2(3)
O(3W)-Co(1)-O(1W)	92.6(3)		

Table 6: The bond lengths (Å) and bond angles around Mo and Co center in compound 2b

Mo(1)-O(1)	1.690(7)	Mo(1)-O(2)	1.679(7)
Mo(1)-O(3)	1.894(7)	Mo(1)-O(4)	2.076(8)
Mo(1)-O(6)	2.185(7)	Mo(2)-O(8)	1.702(9)
Mo(2)-O(9)	1.714(8)	Mo(2)-O(10)	1.869(8)
Mo(2)-O(11)	2.021(7)	Mo(2)-O(13)	2.197(10)
Mo(1)-N(1)	2.348(8)	Mo(2)-N(2)	2.307(9)
Co(1)-O(1W)	2.080(14)	Co(1)-O(2W)	2.065(10)
Co(1)-O(3W)	2.131(8)	Co(1)-O(4W)	2.099(10)
Co(1)-O(7)	2.095(8)	Co(1)-O(20)	2.064(15)

Angles around Mo-center

O(2)-Mo(1)-O(1)	106.0(4)	O(2)-Mo(1)-O(3)	98.7(3)
O(1)-Mo(1)-O(3)	105.2(4)	O(2)-Mo(1)-O(4)	90.8(3)
O(1)-Mo(1)-O(4)	94.7(3)	O(3)-Mo(1)-O(4)	154.5(3)
O(2)-Mo(1)-O(6)	163.2(3)	O(1)-Mo(1)-O(6)	89.5(4)
O(3)-Mo(1)-O(6)	83.2(3)	O(4)-Mo(1)-O(6)	81.1(3)
O(2)-Mo(1)-N(1)	91.2(3)	O(1)-Mo(1)-N(1)	158.3(3)

O(3)-Mo(1)-N(1)	84.6(3)	O(4)-Mo(1)-N(1)	71.5(3)
O(6)-Mo(1)-N(1)	72.2(3)	O(8)-Mo(2)-O(9)	105.5(4)
O(8)-Mo(2)-O(10)	103.4(4)	O(9)-Mo(2)-O(10)	99.1(4)
O(8)-Mo(2)-O(11)	95.4(4)	O(9)-Mo(2)-O(11)	91.1(3)
O(10)-Mo(2)-O(11)	155.3(3)	O(8)-Mo(2)-O(13)	90.6(4)
O(9)-Mo(2)-O(13)	162.6(4)	O(10)-Mo(2)-O(13)	83.1(4)
O(11)-Mo(2)-O(13)	80.7(3)	O(8)-Mo(2)-N(2)	162.3(4)
O(9)-Mo(2)-N(2)	89.5(4)	O(10)-Mo(2)-N(2)	83.0(3)
O(11)-Mo(2)-N(2)	74.5(3)	O(13)-Mo(2)-N(2)	73.5(3)

Angles around Co center

O(2W)-Co(1)-O(20)	93.5(6)	O(2W)-Co(1)-O(1W)	88.0(7)
O(20)-Co(1)-O(1W)	178.5(7)	O(2W)-Co(1)-O(7)	94.0(3)
O(20)-Co(1)-O(7)	90.3(4)	O(1W)-Co(1)-O(7)	89.1(5)
O(2W)-Co(1)-O(4W)	175.7(6)	O(20)-Co(1)-O(4W)	90.0(6)
O(1W)-Co(1)-O(4W)	88.6(7)	O(7)-Co(1)-O(4W)	88.6(4)
O(2W)-Co(1)-O(3W)	85.7(4)	O(20)-Co(1)-O(3W)	87.9(4)
O(1W)-Co(1)-O(3W)	92.7(4)	O(7)-Co(1)-O(3W)	178.1(4)
O(4W)-Co(1)-O(3W)	91.9(4)		

Table 7: The bond lengths (Å) and bond angles around Mo and Co center in compound 3

Mo(1)-N(1)	2.336(4)	Mo(2)-N(2)	2.329(5)
Mo(1)-O(1)	1.710(4)	Mo(1)-O(2)	1.699(4)
Mo(1)-O(3)	1.886(4)	Mo(1)-O(4)	2.040(5)
Mo(1)-O(6)	2.158(4)	Mo(2)-O(8)	1.701(5)
Mo(2)-O(9)	1.705(5)	Mo(2)-O(10)	1.894(5)
Mo(2)-O(11)	2.071(5)	Mo(2)-O(13)	2.150(4)

Co(1)-O(1W)	2.059(5)	Co(1)-O(2W)	2.129(4)
Co(2)-O(3W)	2.087(5)	Co(2)-O(4W)	2.123(5)
Co(2)-O(5W)	2.090(4)	Co(1)-O(7)	2.105(4)
Co(1)-O(1W)[a]	2.059(5)	Co(1)-O(7)[a]	2.105(4)
Co(1)-O(2W)[a]	2.129(4)	Co(2)-O(3W)[b]	2.087(5)
Co(2)-O(5W)[b]	2.090(4)	Co(2)-O(4W)[b]	2.123(5)

Angles around Mo-center

O(1)-Mo(1)-O(3)	102.1(2)	O(1)-Mo(1)-O(4)	96.3(2)
O(1)-Mo(1)-O(6)	91.5(2)	O(2)-Mo(1)-O(1)	106.5(2)
O(2)-Mo(1)-O(3)	98.7(2)	O(2)-Mo(1)-O(4)	92.9(2)
O(2)-Mo(1)-O(6)	161.13(18)	O(3)-Mo(1)-O(4)	154.44(18)
O(3)-Mo(1)-O(6)	82.80(19)	O(4)-Mo(1)-O(6)	79.04(18)
O(1)-Mo(1)-N(1)	163.1(2)	O(2)-Mo(1)-N(1)	88.00(18)
O(3)-Mo(1)-N(1)	83.80(16)	O(4)-Mo(1)-N(1)	73.89(16)
O(6)-Mo(1)-N(1)	73.41(15)	O(8)-Mo(2)-O(9)	105.7(3)
O(8)-Mo(2)-O(10)	100.0(3)	O(8)-Mo(2)-O(11)	89.7(2)
O(8)-Mo(2)-O(13)	162.1(2)	O(9)-Mo(2)-O(10)	105.4(2)
O(9)-Mo(2)-O(11)	93.8(2)	O(9)-Mo(2)-O(13)	89.2(2)
O(10)-Mo(2)-O(11)	155.12(18)	O(10)-Mo(2)-O(13)	85.2(2)
O(11)-Mo(2)-O(13)	79.3(2)	O(8)-Mo(2)-N(2)	89.3(2)
O(9)-Mo(2)-N(2)	160.7(2)	O(10)-Mo(2)-N(2)	83.30(18)
O(11)-Mo(2)-N(2)	73.85(17)	O(13)-Mo(2)-N(2)	74.13(16)
C(7)-N(1)-Mo(1)	107.7(3)	C(8)-N(1)-Mo(1)	102.8(3)
C(10)-N(1)-Mo(1)	112.4(3)	C(26)-N(2)-Mo(2)	107.9(4)
C(27)-N(2)-Mo(2)	104.6(4)	C(29)-N(2)-Mo(2)	110.9(3)
C(1)-O(3)-Mo(1)	139.8(4)	C(9)-O(4)-Mo(1)	121.5(4)
C(11)-O(6)-Mo(1)	123.7(4)	C(20)-O(10)-Mo(2)	140.4(4)
C(28)-O(11)-Mo(2)	123.1(4)	C(30)-O(13)-Mo(2)	123.2(4)

Angles around Co center

O(1W)-Co(1)-O(1W)^a	180.0(3)	O(1W)-Co(1)-O(7)	91.23(19)
O(1W)^a-Co(1)-O(7)	88.77(19)	O(1W)-Co(1)-O(7)^a	88.77(19)
O(1W)^a-Co(1)-O(7)^a	91.23(19)	O(7)-Co(1)-O(7)^a	180.00(18)
O(1W)-Co(1)-O(2W)	92.1(2)	O(1W)^a-Co(1)-O(2W)	87.9(2)
O(7)-Co(1)-O(2W)	95.13(16)	O(7)a-Co(1)-O(2W)	84.87(16)
O(1W)-Co(1)-O(2W)^a	87.9(2)	O(1W)^a-Co(1)-O(2W)^a	92.1(2)
O(7)-Co(1)-O(2W)^a	84.87(16)	O(7)^a-Co(1)-O(2W)^a	95.13(16)
O(2W)-Co(1)-O(2W)^a	180.0(1)	O(3W)-Co(2)-O(3W)^b	180.0(1)
O(3W)-Co(2)-O(5W)^b	88.58(18)	O(3W)^b-Co(2)-O(5W)^b	91.42(18)
O(3W)-Co(2)-O(5W)	91.42(18)	O(3W)^b-Co(2)-O(5W)	88.58(18)
O(5W)^b-Co(2)-O(5W)	180.0(1)	O(3W)-Co(2)-O(4W)^b	91.0(2)
O(3W)^b-Co(2)-O(4W)^b	89.0(2)	O(5W)^b-Co(2)-O(4W)^b	90.6(2)
O(5W)-Co(2)-O(4W)^b	89.4(2)	O(3W)-Co(2)-O(4W)	89.0(2)
O(3W)^b-Co(2)-O(4W)	91.0(2)	O(5W)^b-Co(2)-O(4W)	89.4(2)
O(5W)-Co(2)-O(4W)	90.6(2)	O(4W)^b-Co(2)-O(4W)	180.0(2)

Symmetry transformations used to generate equivalent atoms:

a; -x,-y,-z+1 b; -x,-y+1,-z+1

Figures

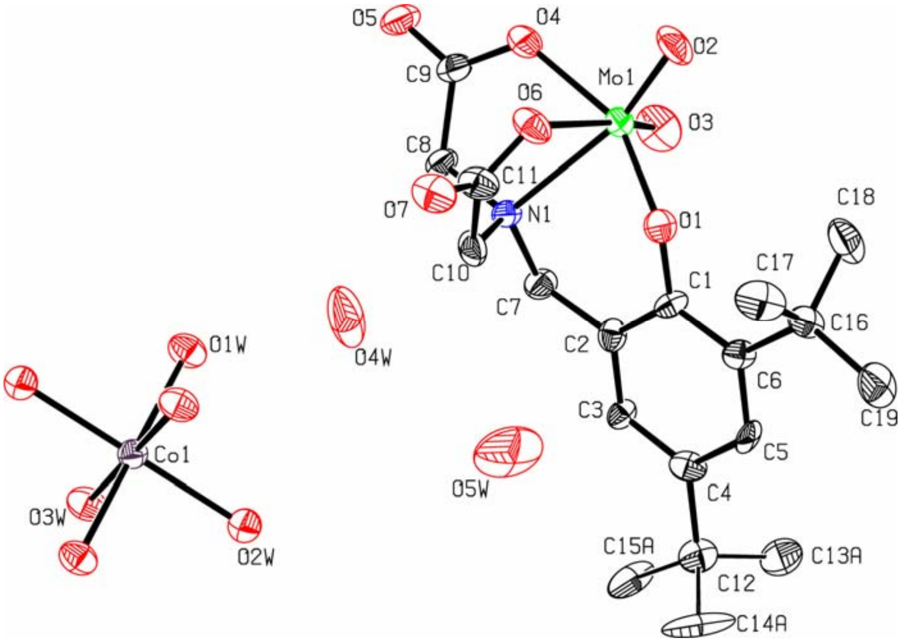


Figure S1 ORTEP plot of **1** with thermal ellipsoid at 30% probability label.

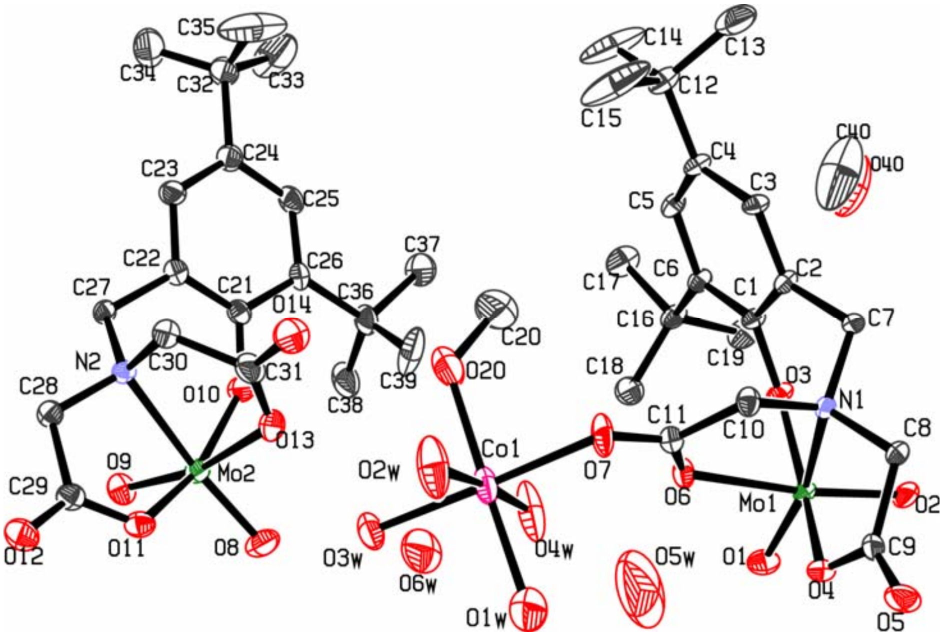


Figure S2 ORTEP plot of **2a.** Thermal ellipsoid drawn at 30% probability label.

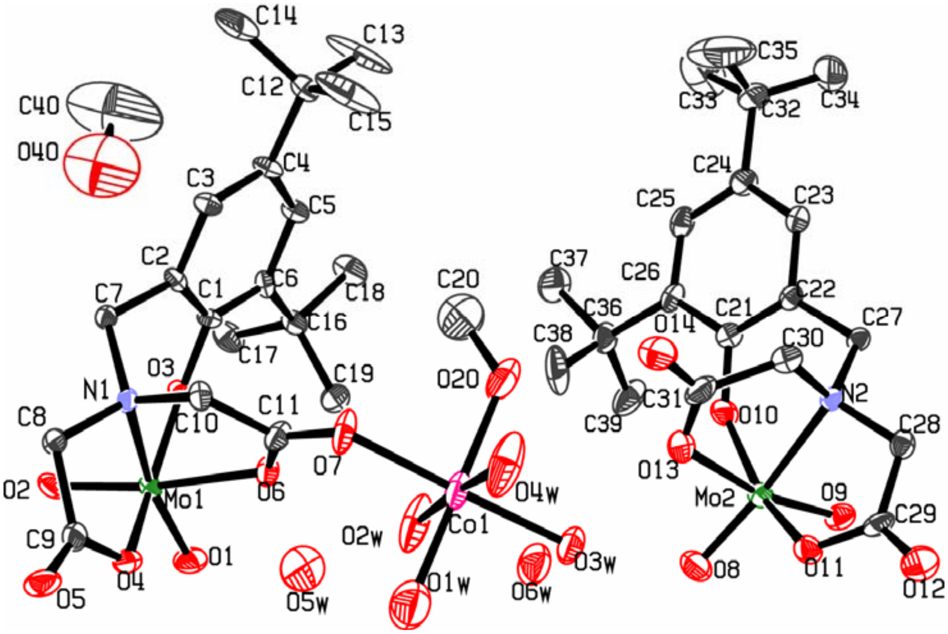


Figure S3 ORTEP plot of **2b.** Thermal ellipsoid drawn at 30% probability label.

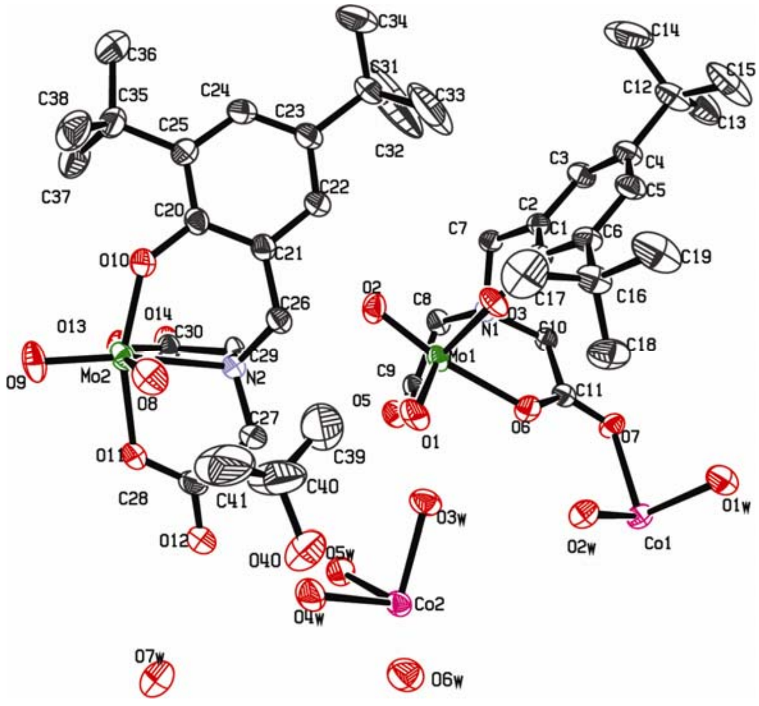
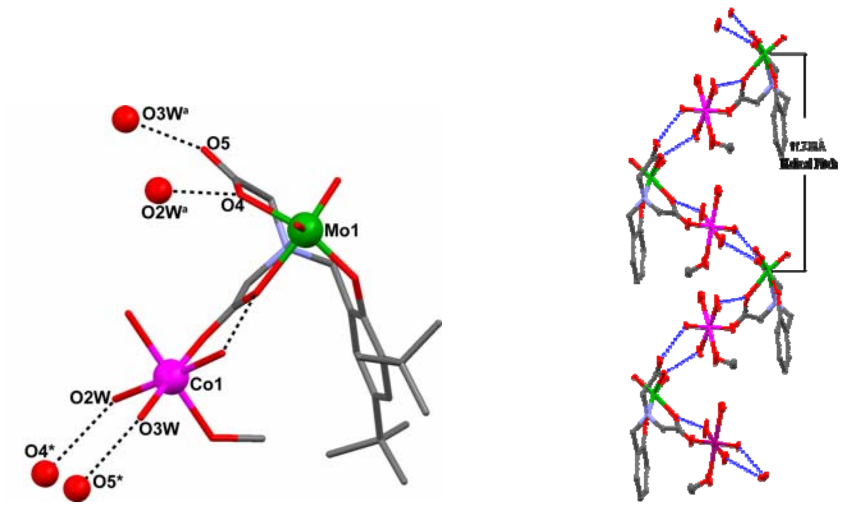
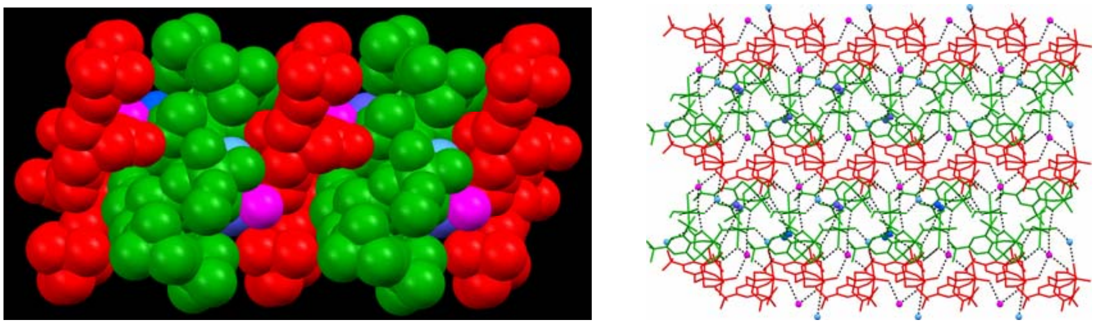


Figure S4 ORTEP plot of **3** with thermal ellipsoid at 30% probability label.



(a) **(b)**

Figure S5 (a) View of the Co(II) coordinated metalloligand unit, $[(MoO_2L)Co(H_2O)_4\text{-}(MeOH)]^+$. This chiral heterobimetallic unit, $[(MoO_2L)Co(H_2O)_4(MeOH)]^+$ acts as both hydrogen bond donor (O2W and O3W) and acceptor (O4 and O5) and forms right handed helical chain (*P*-Helical) in **2a**. Amabilino *et al* recently reported this type of unit as “enantiophobic” unit[9]. (b) View of the formation of H-bonded *P*-helical chain in **2a**. Dotted line; H-bonding.



(a) **(b)**

Figure S6 (a) Space filling **v**iew of the hydrogen bonded 2D packing in **2a** along *b* - axis**.** (b) View of the 2D hydrogen bonded network along *c* - axis. Green: Helical chain of heterobimetallic $[(MoO_2L)Co(H_2O)_4(MeOH)]^+$ unit where the metalloligand unit is clockwise (*C*). Red: Helical Chain of free anticlockwise (*AC*) metalloligand, $[MoO_2L]^-$. Blue: solvent MeOH; Light blue: O5W; Pink: O6W

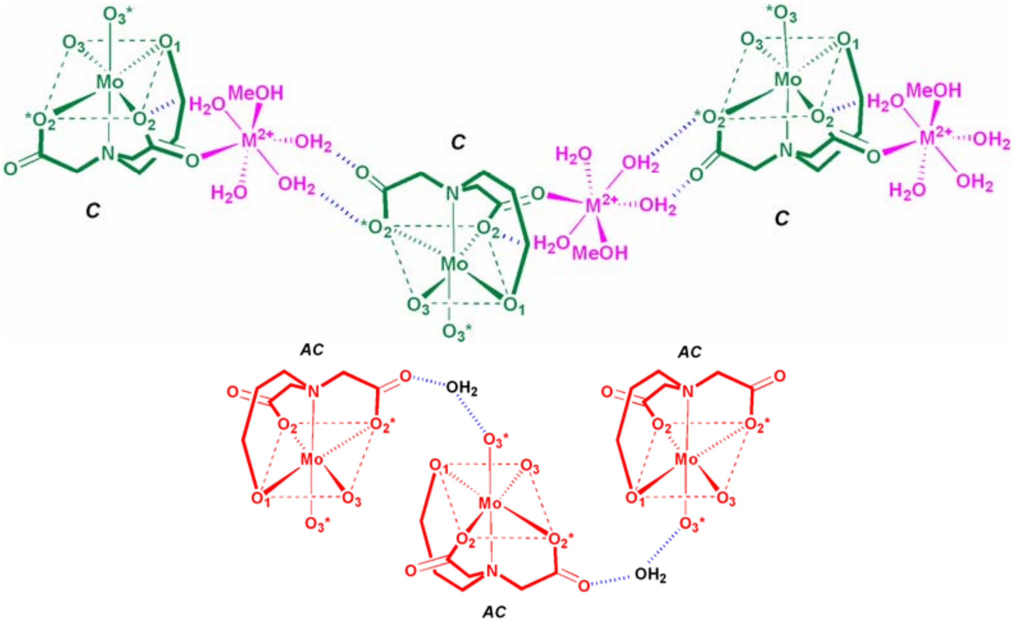


Figure S7: Schematic representation of the formation of heterobimetallic right handed helical chain (Top) and right handed helical chain of free metalloligand (Bottom) in **2a.** Where M = Co

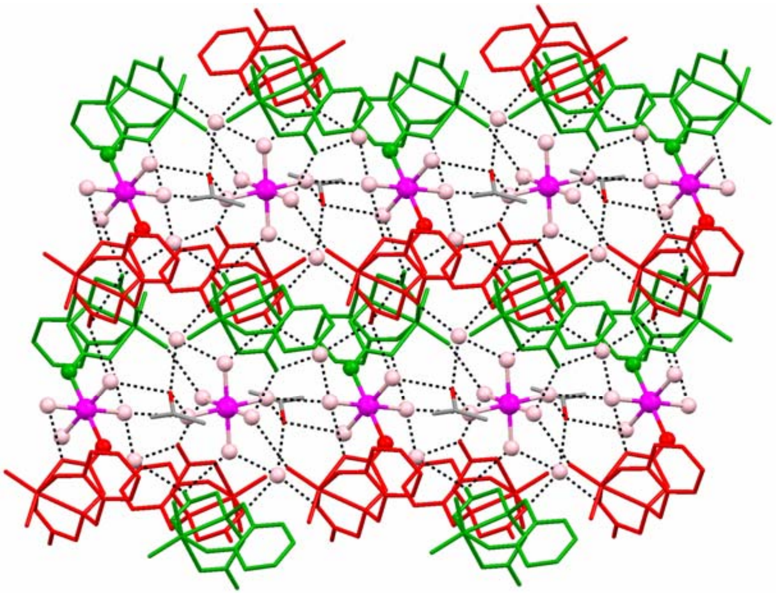
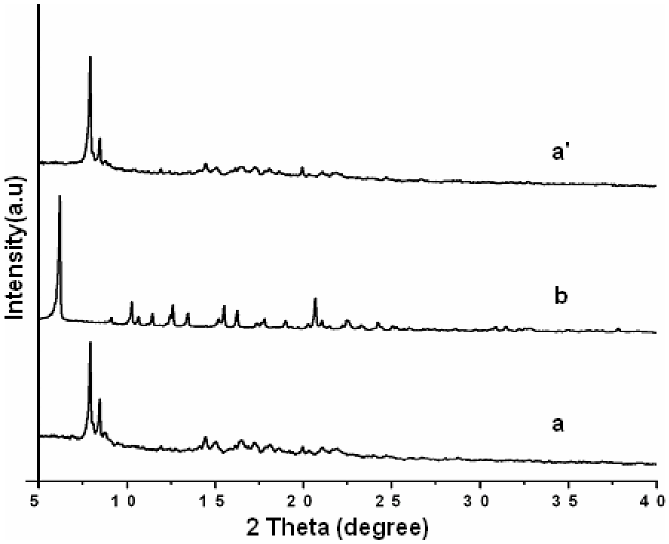


Figure S8 View of hydrogen bonded 2D network in **3** along crystallographic *b*-axis. Pink: Co; Pale pink: coordinated aqua ligand; Green: Clockwise metalloligand; Red: Anticlockwise metalloligand; Black dotted line: H-Bonding. $[Co(H_2O)_6]^{2+}$ shown as ball & stick.

Powder X-Ray Diffraction (PXRD) Study



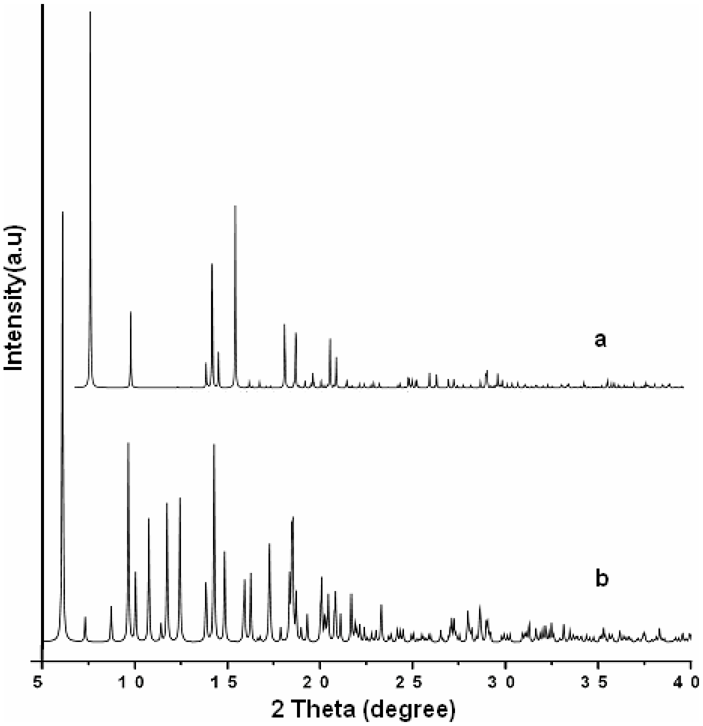
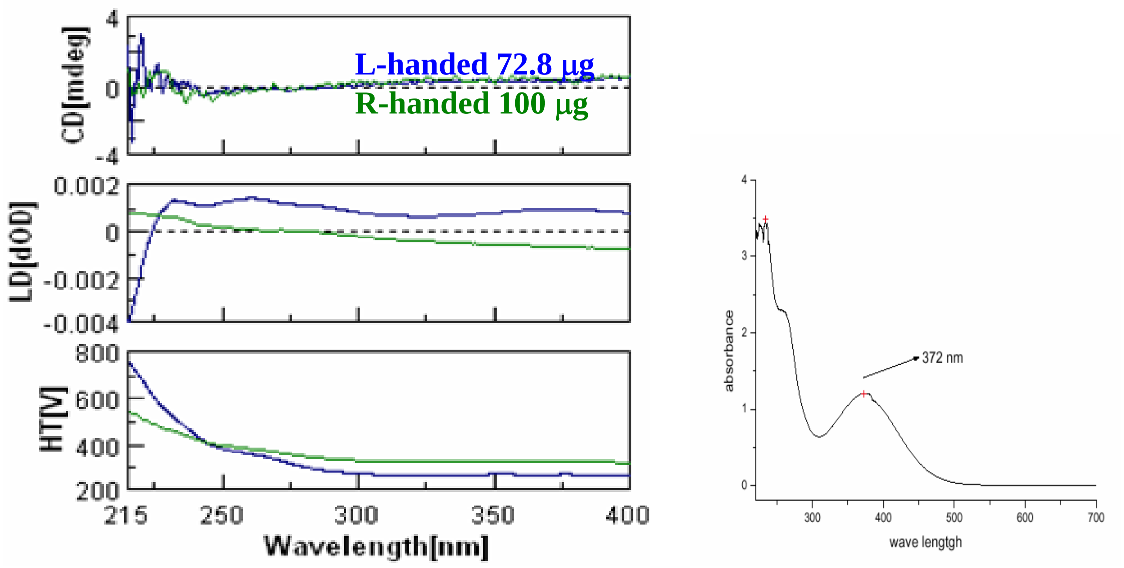


Figure S9 (Top) Powder XRD pattern of, a: compound **1** obtained initially from the reaction mixture, b: compound **2**, a': compound **1** obtained by the recrystallization of **2** from aqueous methanol (4:1) at pH ~ 3. (Bottom) Simulated powder XRD pattern of a: compound **1** and b: compound **2**

CD measurements of compound 2 (a and b) in the solid state:



(a) **(b)**

Figure S10 a) Transmittance CD spectra of a KBr disk made with a chiral right handed **2a** (green) and left handed **2b** (blue) single crystal (72.8 and 100 µg for the (L)-handed and (R)-handed crystals, respectively) co-ground with KBr matrix. b) UV-Vis spectrum of the compound **2** in the solution state.

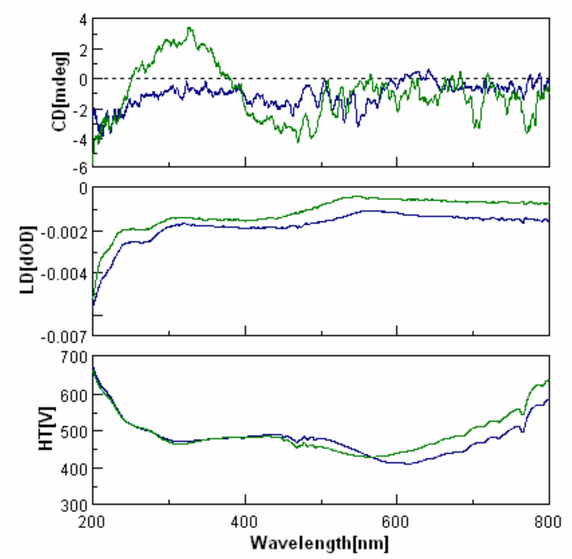


Figure S11 DRCD spectra of chiral **2a** and **2b** powdered samples on a quartz plate [(L)-handed crystal **2b** (green), (R)-handed crystal **2a** (blue)].

Thermogravimetric Analyses:

The thermogravimetric analyses (TGA) of compound **2**, and **3** (crystal) have been performed in air in the temperature range of 50 to 650 ºC**.** The total weight loss from 50 °C to 510°C can associated with the loss of six water molecules (4 coordinated and 2 solvent) two methanol and two organic ligands (weight loss: exptl. 69.64 %, calcd. 73.36 %). The 3.72% difference between the calculated weight loss and the observed weight loss is due to the remaining three oxygens which are used to form the residue. The residual weight, 30.36%, (calculated: 30.65 %) corresponds to mixed bimetallic oxide of the formula $CoO{\cdot}2MoO_3$. The thermal decomposition pattern of **3** shows that the total weight loss from 50°C to 530°C can associated with the loss of fourteen water molecules (10 coordinated and 4 solvent) two iso-propanol and four organic ligands (weight loss: exptl. 69.65 %, calcd. 73.67 %). The 4.02% difference between the calculated weight loss and the observed weight loss is due to the remaining three oxygens which are used to form the residue. The residual weight, 30.35%, (calculated: 30.289 %) corresponds to mixed bimetallic oxide of the formula $2CoO{\cdot}4MoO_3$.

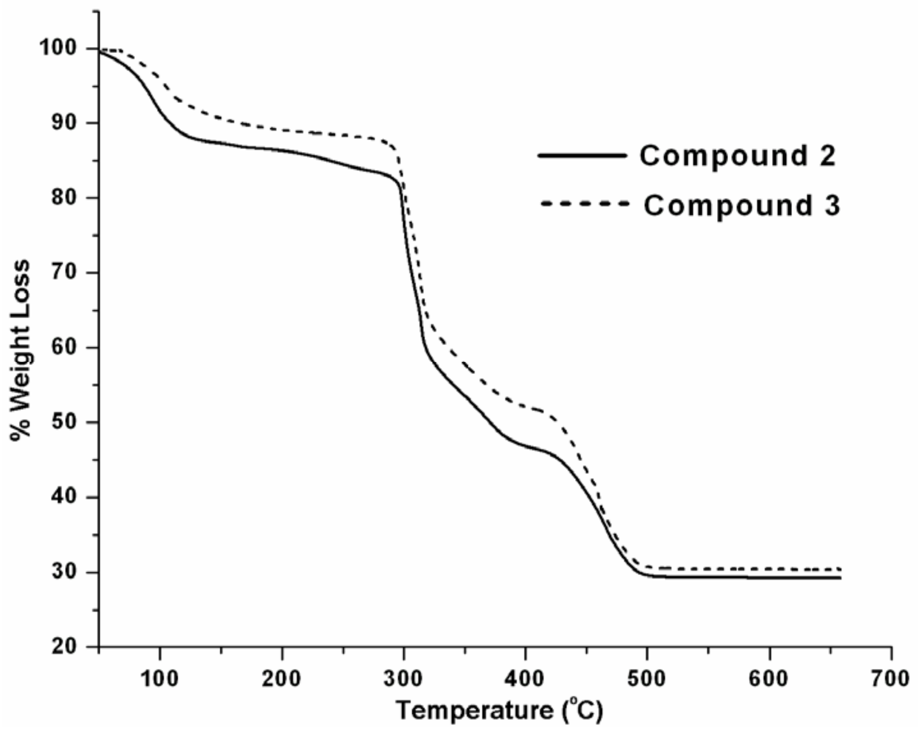


Figure S12: TGA curves of the compound **2** and **3**

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